SUPPORTING INFORMATION

Interfacial Reactions of Ozone with Surfactant Protein B in a Model Lung Surfactant System

Hugh I. Kim[a], Hyungjun Kim[b], Young Shik Shin[c], Luther W. Beegle[a], Seung Soon Jang[d], Evan L. Neidholdt[c], William A. Goddard[b], James R. Heath[c], Isik Kanik[a], and J. L. Beauchamp[c,]*

[a]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109,

[b]Materials and Process Simulation Center, Beckman Institute, California Institute of Technology, Pasadena, CA 91125,

[c]Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, CA 91125,

[d]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0245

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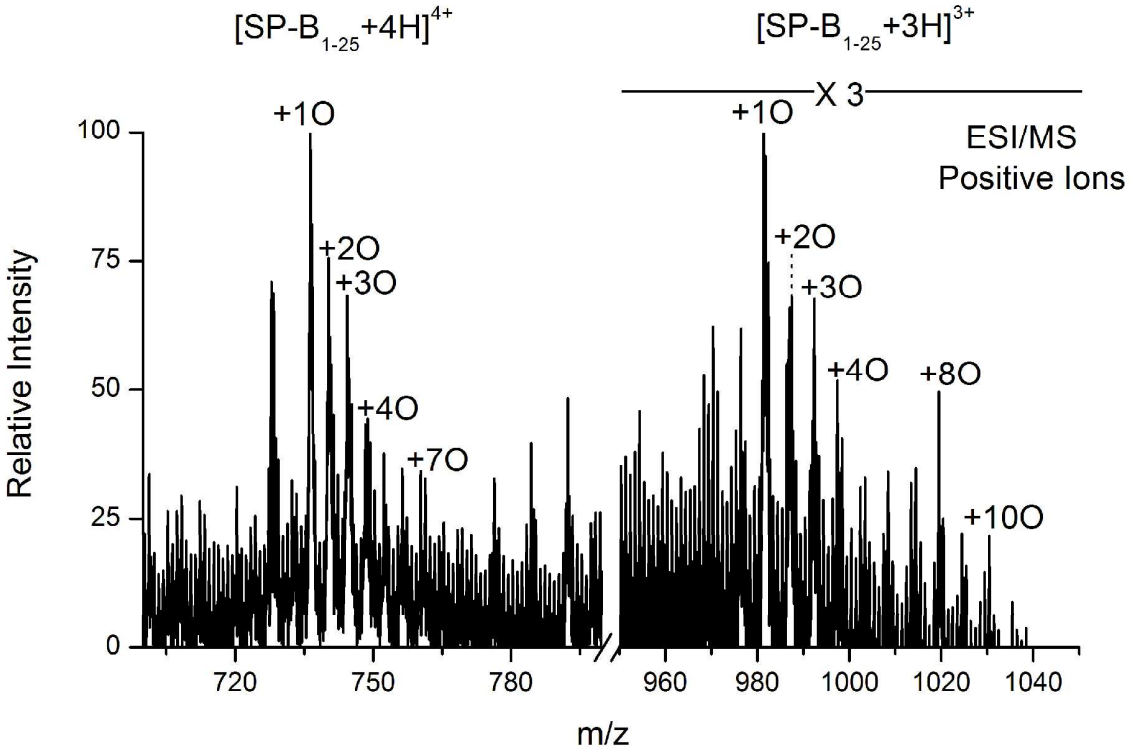

Figure S1. Quadruply and triply charged products from the Fenton reaction with intact SP-B_{1-25}.

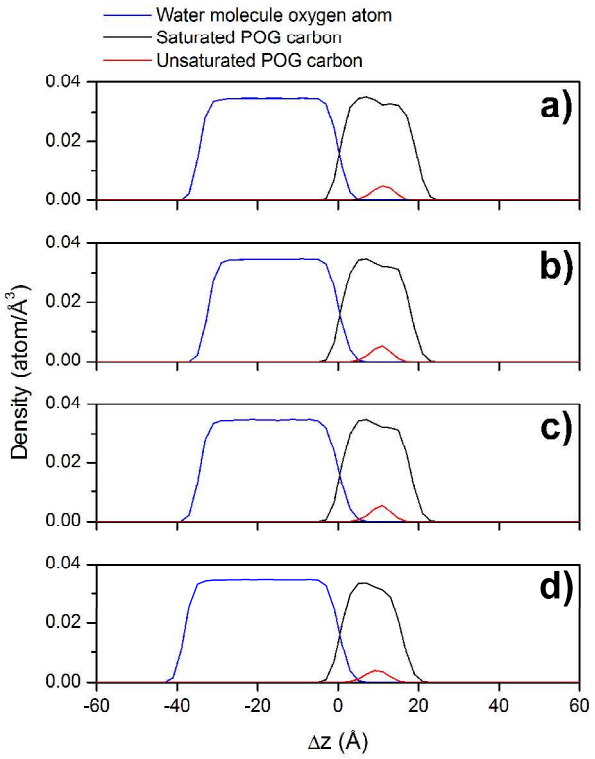

Figure S2. Atomic density profiles of POG monolayer systems as a function of Δz, proceeding left to right from the water to the lipid layer, where the air/liquid interface is at 0. The lipid surface densities are (a) 55 Å^2/lipid, (b) 60 Å^2/lipid, (c) 65 Å^2/lipid, and (d) 70 Å^2/lipid. Blue lines denote the density profiles of the oxygen atoms of water molecules, black lines denote that of saturated carbons of lipid acyl chains, and red lines denote that of unsaturated carbons of lipid acyl chains.

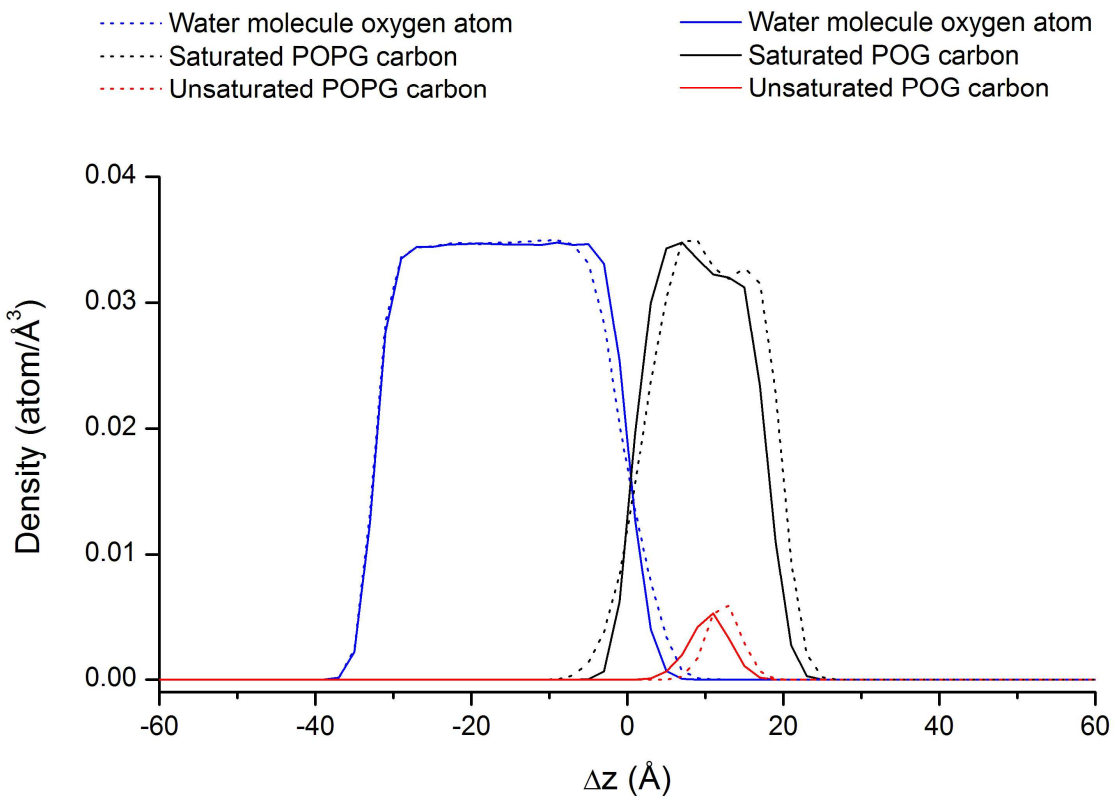

Figure S3. Atomic density profiles of POPG monolayer systems (dotted lines) and POG monolayer systems (solid lines) as a function of Δz, proceeding left to right from the water to the lipid layer, where the air/liquid interface is at 0. The lipid surface density is 60 $Å^2$/lipid. Blue lines denote the density profiles of oxygen atoms of water molecules, black lines denote that of saturated carbons of lipid acyl chains, and red lines denote that of unsaturated carbons of lipid acyl chains.

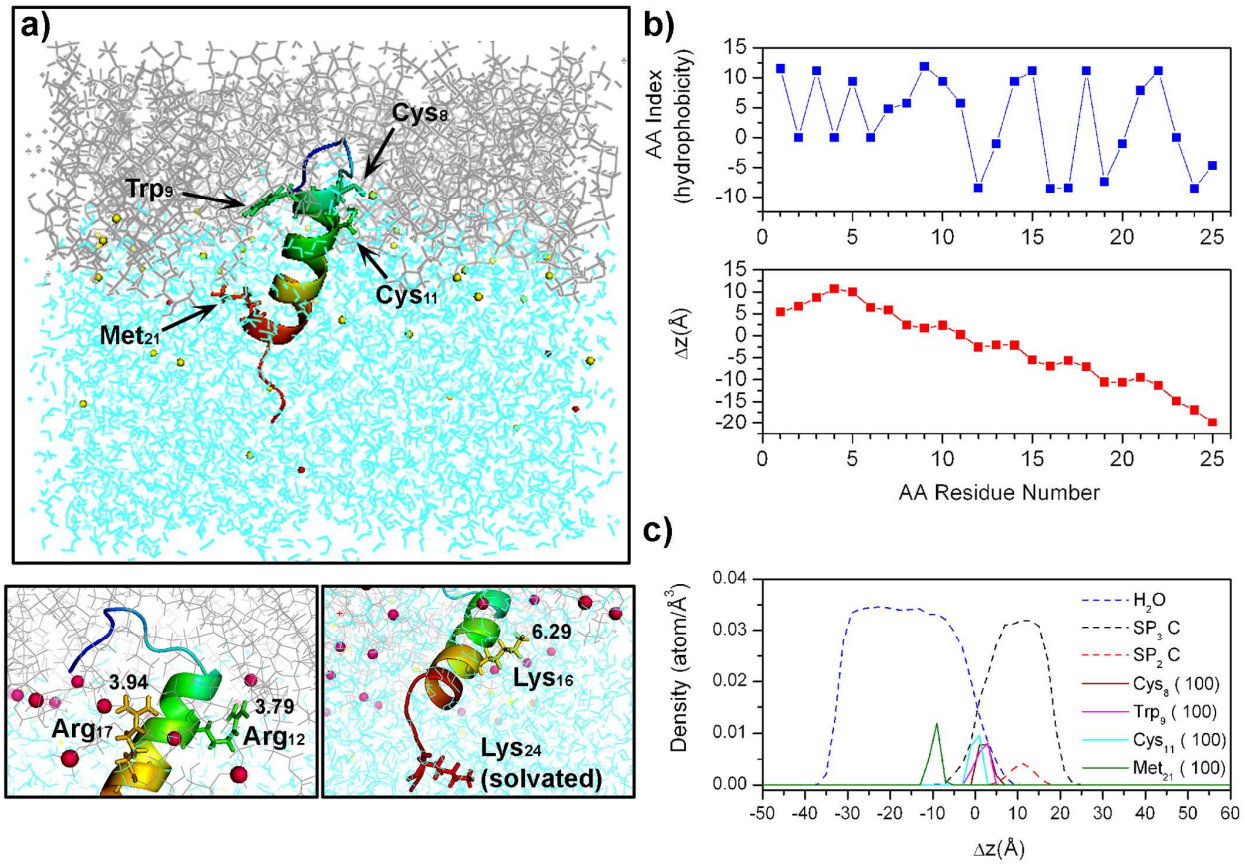

Figure S4. (a) Final snapshot after 2.0 ns MD simulation of SP-$B_{1\text{-}25}$ in POPG monolayer at 60 $Å^2$/lipid is shown at top panel. The peptide is shown in rainbow color (C-terminal: red, N-terminal: blue), lipids in gray, water molecules in cyan, and chloride ions in red. The lower left and right show that Arg residues and Lys residues (displayed with sticks) are interacting with phosphate groups of lipids, respectively. (Phosphorous atoms are in magenta.) (b) AA index for hydrophobicity scale[53] (top) and Δz of C_α of each residue averaged from the last 0.5 ns trajectory of 2.0 ns duration MD simulations (bottom) are plotted as a function of amino acid residue number. The air/water interface is located near Δz = 0. (c) Atomic density profiles of SP-$B_{1\text{-}25}$ in POG monolayer at 60 $Å^2$/lipid as a function of Δz from the last 0.5 ns of the 2.0 ns MD simulation. Blue dash line denotes the density profiles of oxygen atoms of water molecules. Black and red dash lines denote those of saturated and unsaturated carbons of lipid acyl chains, respectively. Wine, magenta, cyan, and olive solid lines denote the 100 times scaled density profiles of the C_α carbon of Cys_8, Trp_9, Cys_{11}, and Met_{21} residues, respectively.

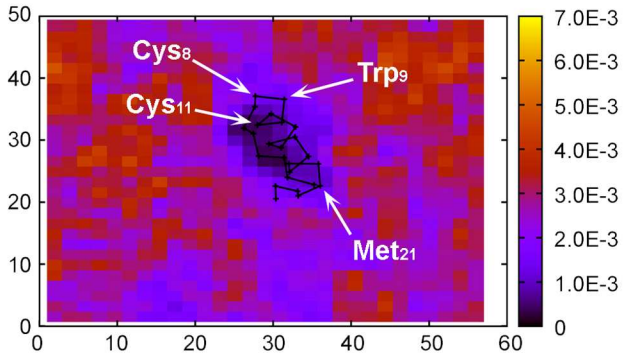

Figure S5. The xy-projected density profiles of saturated carbon atoms of lipid acyl chains is shown with colors and the averaged positions of C_α carbons of SP-$B_{1\text{-}25}$ in the POPG monolayer is indicated by a black line (each residue is shown with cross).

Complete Ref. (35) MacKerell, A. D.; Bashford, D.; Bellott, M.; Dunbrack, R. L.; Evanseck, J. D.; Field, M. J.; Fischer, S.; Gao, J.; Guo, H.; Ha, S.; Joseph-McCarthy, D.; Kuchnir, L.; Kuczera, K.; Lau, F. T. K.; Mattos, C.; Michnick, S.; Ngo, T.; Nguyen, D. T.; Prodhom, B.; Reiher, W. E.; Roux, B.; Schlenkrich, M.; Smith, J. C.; Stote, R.; Straub, J.; Watanabe, M.; Wiorkiewicz-Kuczera, J.; Yin, D.; Karplus, M. *J. Phys. Chem. B* **1998**, *102*, 3586-3616.